

# Imidazole, 1-(p-nitrophenyl)-

<b>Other names:</b>	1-(4-Nitrophenyl)-1H-imidazole 1H-Imidazole, 1-(4-nitrophenyl)- 1-(4-Nitrophenyl)imidazole
<b>Inchi:</b>	InChI=1S/C9H7N3O2/c13-12(14)9-3-1-8(2-4-9)11-6-5-10-7-11/h1-7H
<b>InchiKey:</b>	PUCOOPJLAXJKOO-UHFFFAOYSA-N
<b>Formula:</b>	C9H7N3O2
<b>SMILES:</b>	O=[N+][O-]c1ccc(-n2ccnc2)cc1
<b>Mol. weight [g/mol]:</b>	189.17
<b>CAS:</b>	2301-25-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	1.780		Crippen Method
mcvol	131.830	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2301259&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2301259&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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